

UNIVERSITY OF SASSARI DEPARTMENT OF AGRICULTURAL SCIENCES

Master's Degree in Agricultural Systems Curriculum "Precision agriculture"

Nitrogen fertilization and greenhouse gas emissions: exploring the potential of mitigation through precision agriculture

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Abstract

It is estimated that in 2050 the world population will be 9 billion, hence it is of primary importance to ensure food security for the growing population on the same agricultural land through sustainable intensification, i.e. increasing food production without increasing GHG emissions.

This study is focused on the application of the DSSAT crop model on spring barley in Scotland to support the design of nitrogen fertilization based on precision farming principles. The modelling exercise started from the identification of homogeneous management zones based on multi-year field observations and the quantification of N₂O emissions and NO₃ leaching for each yield zone, with the aim of optimizing fertilization to achieve high yields with substantially reduced emissions at field scale.

The simulations proved that 80 N treatment was very effective vs. the business as usual fertilization rate (120 N) by maitaining crop yield reduction within -5% but reducing nitrate leaching by between -41% and -51% and N_2O gas emissions by between -48% and -50% in relation to the management zone. However, given the relatively homogeneous field conditions, the model output showed negligible advantages from a precision fertilization approach vs. the homogeneous distribution of the optimal N fertilization rate.

Foreword

This thesis is the outcome of my internship project carried out at the James Hutton Institute (JHI), Dundee, Scotland (UK). The experience was made possible thanks to the ERASMUS Traineeship Program. This experience gave me the opportunity to gain new specific skills in on crop modelling and precision agriculture.

Dr. Davide Cammarano supervised my activity during the internship, that included the use of simulation models applied to precision agricultural systems, a field data collection campaign and the calibration and evaluation of the DSSAT model to a specific case study. Dr. Cammarano is a worldwide recognized expert in crop modelling, precision agriculture, agronomy, climate change science, crop and soil, remote sensing and climate forecasting in agriculture. His research focus concerns the impact of climate change on a local and regional scale in a context of transdisciplinary research on agricultural systems in different environmental and socio-economic contexts.

During the time spent in Scotland, I learned how to calibrate and run DSSAT and how to analyse and manage big data.

The activities carried out during the training activity were part of research projects carried out at JHI. Some of the achieved results during the experiment described in this thesis were published in two international peer reviewed ISI journals^{1,2}.

¹ Cammarano D. (a), Hawes C., Squire G., Holland J., Rivington M., Murgia T., Roggero P.P., Fontana F., Casa R., Ronga D., 2019a. Rainfall and temperature impacts on barley (*Hordeum vulgare* L.) yield and malting quality in Scotland. Field Crops Research 241.

² Cammarano D. (b), Holland J., Basso B., Fontana F., Murgia T., Lange C., Taylor J., Ronga D., 2019b. Integrating geospatial tools and a crop simulation model to understand spatial and temporal variability of cereals in Scotland. Precision Agriculture 19, 29-35.

1. Introduction

1.1 Digital agriculture

The Agricultural revolution of 1930s to 1960s focused on increasing agricultural production and mechanization. Technology was at the centre of its success. However, 50 years later, there are still many people who are hungry: today 815 million people are chronically undernourished (FAO, 2017). Agricultural systems are therefore asked to satisfy the increasing global demand for food and fibre to ensure food security for a growing population (Foley et al., 2011; Tilman et. al., 2011; West et. al, 2014; Boscaro et al., 2018). The intensification of the current agricultural systems in term of inputs and outputs lead to increasing concerns regarding their impact on the environment (Miller et al., 2007). Nowadays, the world is facing the biggest challenge of producing more food on the same or less land, and by reducing its environmental footprint while keeping farming profitable (Cammarano et al., 2016). Performance (2017) quantified the evolution of the amount of people a farmer can feed in relation to the technology used and gives an indication of the projections for the future, in which people will be fed in a more crowded world and under climate change, as shown in the following figure:

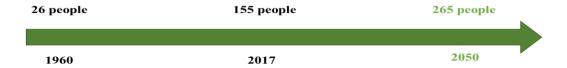


Figure 1 Evolution of the amount of people that a farmer can feed.

Digital Agriculture (DA) plays an important role in reducing agricultural production variability and environmental sustainability in both developed and developing countries as it combines and uses new technologies to increase yields, reduce costs and contribute to maintain a cleaner environment with the global challenge in the context of climate change. DA combines multiple data sources with advanced crop and environmental analyses to

provide support for on-farm decision making (Fulton and Port, 2018) so it could be the next turning point that can address the food security challenge. If DA is fully implemented, it can potentially raise crop production by 70% by 2050 and generate a \$240 billion business in the world economy (Goldman Sachs Group, 2016³). DA combines the latest technologies to increase the overall value of different areas of the farm by translating data into practices to improve profitability and reduce negative environmental footprints.

DA is a component of Internet of Things (IoT) (Fig. 2). IoT is the result of the convergence of sensors, network processing and communication of specialized digital equipment designed to be used wherever it is needed to collect and integrate information and to automate or integrate the operation of different equipment. In agriculture, the IoT makes it possible to computerize and network information, encouraging interaction to support crop management planning.

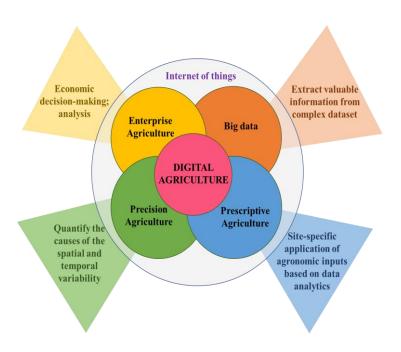


Figure 2 Main components of Digital Agriculture (adapted from Fulton and Port, 2018).

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³ http://www.goldmansachs.com

However, digital technologies will not replace the essential role of the farmer and engineers in the decision-making process. Digital agriculture plays an important role in supplying data to operators. Data collection is the starting point for processing and synthesizing information, which will then be translated into information and then action during production processes. Human decision-making will therefore still be an important factor in monitoring and identifying strategic options for different crop responses.

Information management between/for the different decision-making areas is often carried out by means of company information systems (Mazzetto et al, 2016). Information systems are a set of IT tools that interact each other and help the operator to collect data at the level of each individual production process, and process and store data collected through models and databases. Therefore, information systems include hardware and software components which are divided into interacting subsystems: operational systems and information systems (Pighin and Garzona, 2005). The following table (Table 1) shows the types of data that can be collected to support PA practices.

Table 1 Type of field data that can be collected in the field.

Type of data that can be collected	Description	Example		
Position in the field	A core-technology that identifies real-time position of a vehicle as it moves across a field.	In a tractor equipped with yield monitor and GPS can record yield data that can be plotted in 3D (Longitude; Latitude; Elevation)		
Soil/plant sampling	Sampling is important to gaining better understanding of the properties of the soil / plants at given points.	A sensor can generate spatially variable map but scouting will help to quantify what is the problem.		
Remote sensing	Satellites monitoring; Unmanned Aerial Vehicles (UAV)	Can be used to identify spatial patterns of crop growth or soil variability where subsequent scouting can identify the inherent causes.		
Proximal sensing	Spectral sensors, Machine vision for detection of weeds, TDR technologies	Detect plant vigor, indirectly quantify some soil property		
Weather data	Obtaining a long-term weather series helps to understand the recurrence of certain patterns.	Daily/hourly weather data (e.g. maximum and minimum temperature, rainfall)		
Machine data	Managing crop operations	Fuel use, engine load, application amount		
Yield	Multy-year yield maps	The yield map represents, for a given year, the spatial interactions of soil-time-genotype management from which similar combinations of yield limiting factors can be processed.		

Precision Agriculture (PA) deals with the management of field variability and is therefore a component of DA. PA offers a unique opportunity to achieve such trade-off, but its adoption for agricultural management has been slower than expected due to technological and socioeconomic challenges (Miao et al., 2018). PA or information-based management of agricultural production systems, emerged in the mid-1980s as a tool to apply the right treatment in the right place at the right time (Barrett et al., 2002). It can be also defined as the application of technologies, principles and strategies for management of space and time variability, to increase crop performance and environmental quality (Pierce and Nowak, 1999; Basso et al., 2001; Basso et al., 2007). In fact, assessing variability is the critical first

step in precision agriculture. The processes and properties that regulate crop performance and yield variability in space and time, adequately quantifying the variability of these processes and properties and determining when and where different combinations are responsible for the spatial and temporal variation in crop yield, is the challenge facing precision agriculture (Mulla and Schepers, 1997; Pierce and Novak, 1999).

There are several technologies suggested and developed for precision farming such as GPS guidance system, variable-rate input application, spatial variability monitoring in soil and yield and auto steer technology (Ebel, 2012; Paxton et al., 2011; McKinion et al., 2001). There are already sensors of different types, which can measure soil moisture, micro- and macro-component contents, texture or other soil properties. Such sensors use a variety of measurement techniques (electromagnetic induction, electrical resistivity, ground penetrating radar and gamma sensors, multi- and hyperspectral spectroradiometer and fluorimeter) in conjunction with a global positioning system (GPS) (Castrignanò; et. al, 2018). However, PA is not only "automation" of the processes, but also the need to quickly have adequate information on the phenological and/or phytosanitary states of the crops to plan corrective actions on crop management. The ability to find and use information for management purposes becomes a primary objective for those responsible for running the business (Mazzetto et al, 2016). The aim to integrate the concepts of business management and process automation can better define PA as "a management strategy that uses information technology to collect data from multiple sources with a view to their subsequent use in decisions concerning field production activities" (NRC, 1997).

The causes that make the application of precision farming difficult and not yet widespread is a topic of discussion in the scientific community. The issue is multi-dimensional, as it does not depend only on technical-economic aspects related to the cost of the technology to be used, but also on cultural and social factors for the professional training of operators, who

know how to adequately manage information on the distribution of factors of production and overcome the difficulty concerning the quantitative and qualitative complexity of the data collected. All in a vision of economic feasibility that is difficult to predict and is not always clear.

PA is based on the assessment of within-field variation. Characterizing soil variation quantitatively and locally is crucial to accomplish the objectives of PA because optimum benefits on profitability and environment protection depend on how well land use and agricultural practices match local conditions (Buttafuoco et al., 2017; Castrignanò et al., 2000; Oliver, 2013). One of the greatest obstacles to implement PA derives from the difficulty to accurately determine local variation of agricultural inputs (Evans et al., 1996). An effective solution is offered by using real-time "on-the-go" proximal soil sensors to record soil data at fine spatial resolution (Adamchuk et al., 2004; Viscarra Rossel et al., 2011). To facilitate the management of such variability, management zones (MZs) are delineated. MZs are homogeneous sub-field regions with similar yield-limiting factors or similar attributes affecting yield (Doerge, 1999; Khosla and Shaver, 2001). In this regard, variable rate input (VRI) on stable homogeneous zones promote an increase in crop yield and reduce negative environmental consequences (Basso et al., 2016).

The amount of any agriculture input applied (e.g. fertilizer) may be varied spatially within the field and temporally between years. In fact, for the same field, determination of the optimal amount of any agronomic input should consider site-specific soil properties, current seasonal crop growing conditions and interactions therein (Basso et al, 2011). Spatial variability can be assessed routinely with a variety of tools (e.g. remote sensing, soil sensing) and the overlay of many thematic maps, such as for soil and crop yield, to divide the field into uniform management zones (Miao et al, 2006). Several methods have been proposed to define such zones (Nawar et al., 2017). However, an important step in taking the right

agronomic decision is to quantify which factors cause the main spatial and temporal variability in the field; with the latter component often not receiving enough attention (McBratney et al, 2005). Crop simulation models (CSM) can be used to consider the interannual weather impact on the soil-plant-atmosphere interactions. They seek to simulate the effects and temporal interactions of water and nitrogen on crop growth as affected by weather and agronomic management (Jones et al. 2003). They have been used in a variety of cropping systems and environmental conditions and to quantify the temporal stability of management zones (Basso et a., 2001; Koo and Rivington, 2005).

1.2 Spring barley in Scotland

Barley (*Hordeum vulgare* L.) is one of the most important cereals worldwide and is a key crop for Scotland's agriculture due to its use in distilleries to produce whisky (Cammarano et al. 2019a). There are several uses that can be made with barley: from human and animal feed to the production of alcohols such as whisky and beer. However, for the Scottish distillates industry spring barley is the most important crop.

The spring barley cultivated for distilleries is a two-row barley (*Hordeum disticum L.*). The choice of this species is due to the low protein content (less than 11-12% of DM), which is a prerequisite for high quality malt production. Furthermore, distilleries made a selection of cultivars that have an high germination capacity (95%), high 1000 seeds weight (> 39-40g) and high grain size (more than 60% must have a diameter greater than 2.5 mm). Given these preconditions, they use spring barley for distillation because it satisfies malting requirements. Spring barley is cultivated over 245,000 ha in Scotland, with an average grain yield of 5.9 t ha⁻¹ (RESAS, 2017). The average turnover across all Scottish barley business is some ϵ

1.3 Crop models

Among the disciplines that are most changing the approach to existing problems in agricultural research, the use and expansion of crop growth and development simulation models, certainly play a role of primary importance (Basso et. al, 2016). Crop simulation models can quantify the interaction between multiple stresses and crop growth (Basso et al. 2001; 2011; Batchelor et al., 2002; Schnebelen et al., 2004). They have shown to be useful tools to understand the interaction between soil, climate, genotypes and management over space and time and to design best management practices required for sustainable crop production (Basso and Ritchie, 2015). Furthermore, they are also used to simulate the longterm effects of management approaches of different soils on crop yield, SOC storage, and GHG emissions (Pezzuolo et al., 2017). The systematic approach offered by the models can contribute both to increasing the agricultural income through the reduction of business costs or the increase in unit production and to reducing the environmental impact of the agricultural practices implemented, with a better care to natural resources conservation (Basso et. al, 2005). The simulation models are distinct in deterministic and stochastic models (Table 2). Deterministic models provide results based on exact environmental conditions, the assumption being that plants and soil within the simulated space are uniform. These models can be classified as statistical, mechanistic or functional models. Statistical models cannot be used to predict the impact that new agronomic practices could have over time and space, because the results cannot be extrapolated outside the geographical area or time frame used for calibration. The mechanistic models are based on mathematical formulas that describe the physical, chemical and biological processes that take place in the soil-plant-atmosphere continuum, these require large amounts of data and inputs to be performed. The functional type models use simplified equations and logics to subdivide the total biomass production into its components.

Table 2 Different types of simulation models.

	Statistical	
Deterministic	Machanistic	
	Functional	
Stochastic		

The simulation of a system is defined as the imitation in time of a dynamic process or of the functioning of the system itself and allows the evaluation of a scenario to operate inferences concerning the behaviour of the system. The models need specific input data to simulate the soil-plant-atmosphere system. In general, the most used models require a minimum data set, that is, it is necessary to have a certain number of inputs without which the simulations cannot work. The minimum data set is composed in:

- Coordinates of experimental site
- Daily meteorological data (date, rainfall, Tmax, Tmin, solar radiation)
- Soil data (depth, texture, pH, bulk density and micro- and macro-elements content)
- Sowing (management, number of seeds m⁻², distance between rows, date)
- Fertilization (management, amount kg ha⁻¹, type of fertilize, date)
- Irrigation (management, amount mm ha⁻¹, date)
- Managements in the field
- Cultivar selected.

After the model runs, cultivar needs a calibration to parameterize yield quantities and phenology. Calibration is an effort to better parameterize a model to a given set of local conditions, thereby reducing the prediction uncertainty. Model calibration is performed by carefully selecting values for model input parameters by comparing model output with

observed data for the same conditions. This is necessary to allow the subsequent application of the model in similar systems. Validation is the process of demonstrating that a given site-specific model is capable of making sufficiently accurate simulations.

1.4 Greenhouse gases and N fertilization

Agricultural activities contribute to greenhouse gas (GHG) emissions to the atmosphere. Croplands are both a sink and a source of GHG emissions (Kim et al., 2016). From an economic point of view, the green revolution was certainly a success, but the negative side of it are the effects of production intensification based on higher agronomic inputs. In 2005 agriculture produced between 1.4 and 1.7 Gt (gigatonnes) of greenhouse gases (GHG), corresponding to 10-12% of the total human emissions, which include 0.76 Gt of CO₂equivalent from N₂O (Burney et al., 2016). In addition, the agricultural sector is an indirect cause of emissions in the industrial and energy sectors producing fertilizers and pesticides, the use of energy in the farms and the production and operation of agricultural machinery. Agricultural sector is responsible for a significant fraction of anthropogenic emissions, up to 30% according to the Intergovernmental Panel on Climate Change (IPCC) (FAOSTAT, 2013). GHG emissions are the engine of Climate Change (CC) because they trigger global warming (IPCC AR5). The negative effects of climate change are more evident for the agricultural sector as they involve the variation of precipitation, drought, floods and the redistribution of pests on a global scale (FAO, 2019). CC is having effects on crop and animal yields and processes such as water percolation, nutrient leaching and further emission of greenhouse gases that are highly site-specific (Kersebaum & Nendel, 2014; Nendel et al., 2014). The strategy to address CC issues consists mainly in the combination of adaptation and mitigation practices, intended as reduction of greenhouse gas emissions. In this contest, modelling tools are widely accepted for assessing crop management options or for assessing

the impact of climate change on crop production, food security and ecosystem services (Ewert et al., 2015).

Among the GHGs, nitrogen dioxide (N_2O) is one of the highly reactive gases. The impact of 1g of N_2O on warming the atmosphere is almost 300 times that of 1g of carbon dioxide (EPA) In agriculture one of the causes of N_2O emissions are anthropogenic N inputs. Indeed, in most soils, an increase in available N enhances nitrification and denitrification rates which then increase the emission of N_2O (IPCC, 2006). The environmental conditions that determine the denitrification in the soil are the high temperatures in a reducing environment, for example in a water saturated soil. The IPCC in the 2006 identified the sources of N_2O as:

- synthetic N fertilisers (FSN);
- organic N applied as fertiliser (e.g., animal manure, compost, sewage sludge, rendering waste);
- urine and dung N deposited on pasture, range and paddock by grazing animals;
- N in crop residues (above-ground and below-ground), including from N-fixing crops and from forages during pasture renewal;
- N mineralisation associated with loss of soil organic matter resulting from change of land use or management of mineral soils.

2. Hypotheses and objectives

The hypothesis of this study is that the application of the crop simulation models to precision agriculture can provide a substantial contribution to design effective and efficient spring barley cropping systems for the Scottish malt industry, with particular focus on the control of spatial variation of GHG emissions related to nitrogen fertilization.

The objective of this study was to test the effectiveness of the DSSAT crop model in supporting farmers and advisors for an optimized spatially distributed nitrogen fertilization strategy for spring barley in Scotland that would maximize grain yield while minimizing the GHG emissions per unit product.

The first specific objective was to calibrate DSSAT for the spring barley cropping system grown in Scotland, based on datasets built from the experimental field observations collected during the 2018 growing season.

The second specific objective was to run the simulation with the calibrated DSSAT model, adopting different levels of nitrogen fertilization and analyzing the scenarios in terms of barley yield and GHG emissions to explore the interactions between nitrogen fertilization and soil spatial variability, under irrigated or rainfed conditions.

3. Materials and methods

3.1 Experimental site and data collection.

Two experimental sites were managed during the 2018 growing season: one plot experiment the James Hutton Institute experimental farm and one field experiment in a commercial farm. The experimental site was located at the James Hutton Institute experimental farm (Invergowrie, Dundee, 56° 27′ N 03° 04′ W, 27 m a.s.l.). The soil was classified as Brown Forest Soil – Carpow Association according to Bell and Hipkin (1988). The soil texture was loamy, according to the USDA soil survey (2019). Climate records with information on daily solar radiation, air minimum and maximum temperature and rainfall were available from 1974 to 2018.

The spring barley cultivar used for the experiment was "Concerto". Barley was sown on May 4th 2018 at 360 seeds m⁻² in 2 m x 12 m plots. A 6 m buffer strip was planted with spring barley between irrigated and rainfed plots to avoid confounding effects between treatments. The experiment compares two factors (irrigation and fertilization) each with two levels (Table 3).

Table 3 Combination of treatments applied to spring barley in the 2018 experiment run at the JHI.

TREATMENTS	IRRIGATION (mm week ⁻¹)	FERTILIZATION (kg ha ⁻¹)
+N - IRR	11	120
+N - RF	0	120
0N - IRR	11	0
0N - RF	0	0



Figure 3 The spring barley experimental field at tillering.

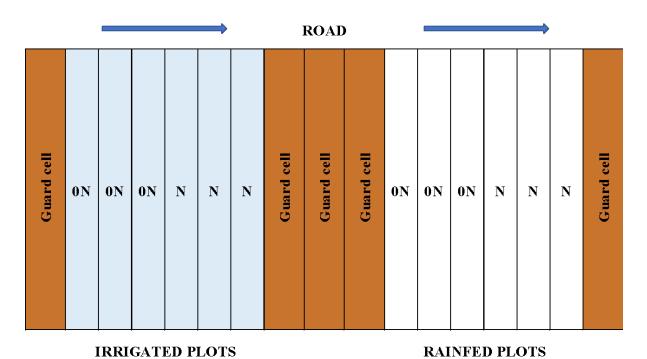


Figure 4 Experimental layout of the spring barley field during the 2018 growing season.

On 17th August 2018, soil cores were collected at three soil depths (0-30 cm, 30-60 cm, 60-90 cm). Plant samples were also collected and oven-dried at 105 °C until constant weight and weighted to measure the aboveground biomass production. At harvest (17th August) samples were collected to measure straw biomass and grain biomass (from 2 m² of biomass in the central plot of each treatment), grain protein, grain N%, seed number (with Marvin seed analyzer), seed weight, and thousand grain weight. Anthesis and maturity dates were also recorded.



Figure 5 Example of soil drilling in the experimental field during the 2018 growing season.



Figure 6 Lab equipments used to determine barley yield and its components.



Figure 7 Seed selection for yield determination.

The field scale (11 ha) measurement campaign was undertaken on a commercial farm located in Scotland (56° 33' N 3° 16' W; 50 m a.s.l). The soil was classified as loamy according to the USDA Soil Taxonomy. Spring barley (cv. Concerto) was sown on 12th April 2018 at 350 plants m⁻². Soil homogeneous zones were identified using six consecutive years of winter wheat and spring barley yield maps generated by a combine harvester equipped with grain yield and GPS sensors. The approach developed by Maestrini and Basso (2018a, 2018b) was used to define four zones shown in the following table:

Table 4 Description of homogeneous yield zones.

Yield zone type	Name	Grain yield class	
	HYZ	High Stable	
Stable	MYZ	Medium Stable	
	LYZ	Low Stable	
Unstable	UYZ	Unstable	

In each zone, a transect of 23 points was identified and in each point soil was sampled at three depths (0-30 cm, 30-60 cm, 60-90 cm). Soil samples were collected to determine mineral N and soil water content, crop samples were collected to measure aboveground

biomass and plant nitrogen content. An unmanned aerial vehicle (UAV) was used to collect data on the crop spectral characteristics on May 23rd.

3.2 Crop modelling

The Decision Support System for Agrotechnology Transfer (DSSAT v4.7) model was used for this study. The DSSAT CSM-Barley was used to simulate barley growth and development (Jones et al., 2003).

The input dataset used for calibration included daily weather, soil characteristics, management data (timing and inputs).

The crop model was calibrated using the 2018 +N-IRR for phenology (anthesis and maturity), crop biomass and grain yield, by adjusting the crop parameters of the model, such as vernalization and photoperiod sensitivity, phyllochron, kernel number per unit canopy weight at anthesis, and standard kernel size under optimum conditions. Firstly, the phenology was calibrated until the model simulated the observed dates for anthesis and maturity by adjusting the parameters of vernalization and photoperiod sensitivity. Next, the biomass accumulation was calibrated by adjusting the phyllochron parameter, and finally grain yield was calibrated. The calibration obtained from +N-IRR was used to simulate barley in all MZs. Following the approach described in Basso et al., (2001; 2011), the DSSAT model was run for different yield stability zones with incremental N amounts (0N, 20N, 40N, 60N, 80N, 100N, 120N-farmers' practice-, 140N) with a daily weather dataset of 35 years(1984-2018). Of the model outputs grain yield, cumulative leaching and cumulative GHG emissions at harvest were considered.

The simulations were conducted in continuum but with restoration of the initial conditions for the soil for each year. The objective was to evaluate yields and emissions by adopting increasing doses of N inputs.

3.3 Statistical analysis

The performance of model in the simulation of was evaluated by calculating complementary indicators. The relative root mean square error (RRMSE) was used to assess the goodness-of-fit between simulated and measured:

$$RRMSE = \frac{\sqrt{\sum i = 1 (y_i - \hat{y}_i)^2}}{\frac{n}{Y}} \cdot 100$$

where y_i are the simulations, \hat{y}_i the observations, n is the number of comparisons and Y is the observations mean. The lowest possible value of RRMSE is zero, when there is no difference between simulated and observed data.

Regression analysis was performed with the MS EXCEL software program. The means of measured yield were regressed against simulated values to test if slopes and intercepts of linear regression were significantly different from 1.0 and 0.0, respectively.

4. Results and discussion

4.1 Cultivar calibration

The simulation of barley phenology for the +N-IRR calibration was very satisfactory (Figure 6). The simulated anthesis date was only one day different from the observed one. The simulated maturity date was the same as the observed one. The observed grain yield was 3500±500 std dev kg dry matter (DM) ha⁻¹, the simulated grain yield was only 240 kg DM ha⁻¹ greater than the observed one. The simulated and measured aboveground biomass (Figs 7, 8, 9 and 10) indicate a satisfactory fitting of the simulated vs. observed values for all the treatments. The model performances were satisfactory as shown in Table 3.

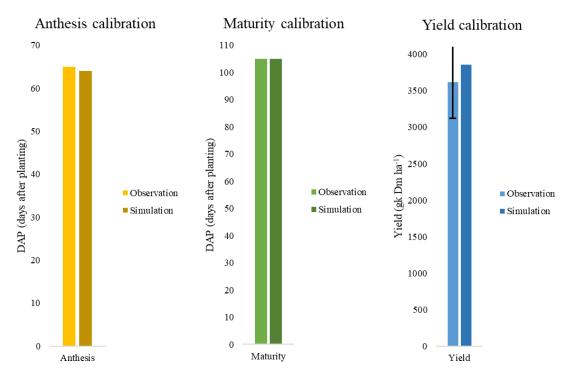


Figure 8 Calibration of the DSSAT model to simulate spring barley (a) anthesis, (b) maturity and (c) grain yield.

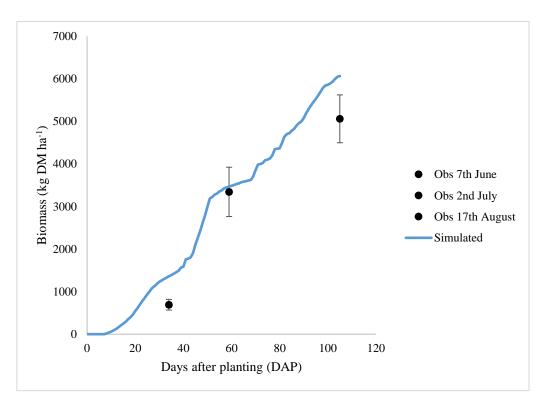


Figure 9 Simulated (blue line) and observed (black dots) crop dry aboveground biomass for the irrigated and fertilized treatment. The vertical lines of observed data represent the standard deviation.

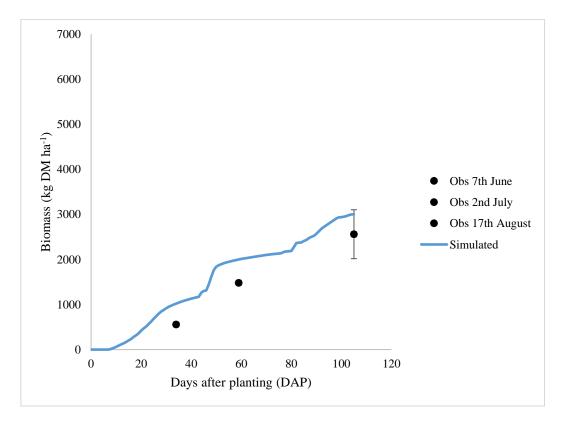


Figure 10 Simulated (blue line) and observed (black dots) crop dry aboveground biomass for the irrigated and rainfed treatment. The vertical lines represent the standard deviation.

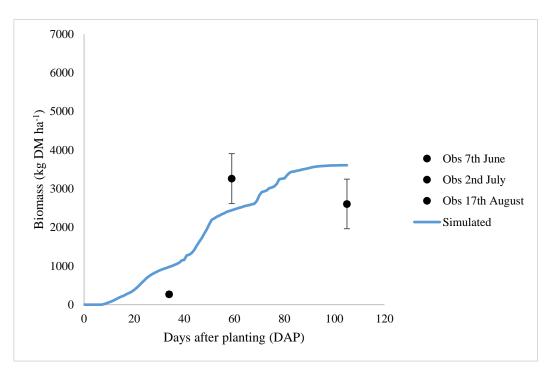


Figure 11 Simulated (blue line) and observed (black dots) crop dry aboveground biomass for the unfertilized and irrigated treatment. The vertical lines represent the standard deviation.

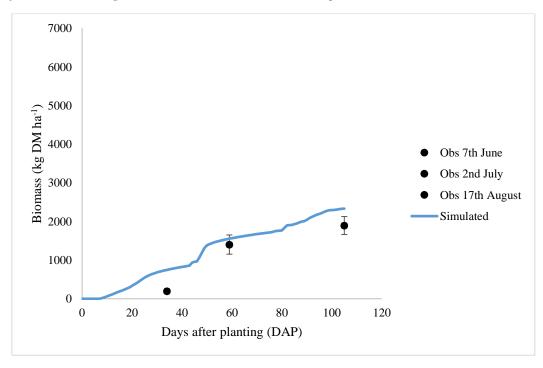


Figure 12 Simulated (blue line) and observed (black dots) crop dry aboveground biomass for the unfertilized and rainfed treatment. The vertical lines represent the standard deviation.

Table 3 Statistical indices to assess simulation efficiency after the calibration.

Parameter	RRMSE	Slope	Intercept	\mathbb{R}^2	Mean Obs	Mean Sim
Min	0.00	-inf.	-inf.	0.00		
Max	+inf.	+inf.	+inf.	1.00		
Best	0.00	1.00	0.00	1.00		
+N-IRR	23.1	1.05	440	0.97	3031	3630
+N-RF	43.0	0.46	1057	0.54	2047	2008
0N-IRR	55.9	1.31	339	0.99	1534	2344
0N-RF	35.8	0.88	517	0.95	1164	1545

4.2 Management zones

The HYZ was mostly concentrated in one portion of the field, while the UYZ was distributed at the edges of the field and the mid-lower part. The LYZ was concentrated in the portion mid-lower at south-west of the field and the MYZ was mainly diffused in the central portion of the field, near the high and low zones (Fig 4). The UAV image (NDVI), collected 22 days after N fertilization, showed how crop growth patterns corresponded with the zones described in Fig 4a. The coloured points on Fig 4b indicate where soil samples were taken in each of the four MZs.

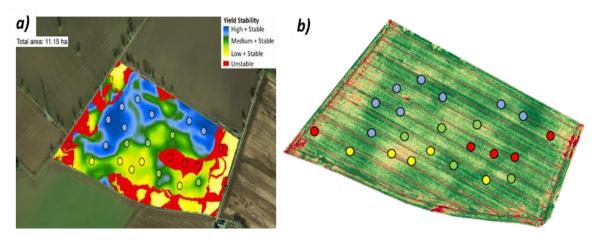


Figure 13 Spatial patterns of the (a) zones and (b) drone image collected on 23^{rd} May with corresponding points sampled in the field (adapted from Cammarano, 2019b).

In most of the soil samplies of the 0-30 cm layer, texture was classified as loamy according to the USDA Soil Taxonomy (Fig 5). In the 30-60 cm and 60-90 cm layer, the texture of the different MZs ranged from clay to sandy loam. Overall, in the 0-30 cm layer, the soil had between 40% to 60% of sand and less than 20% of clay across all the zones, while at depth, the clay content was about 20% and sand content 30% to 40%.

The soil organic carbon (SOC) was close to 1% in the 0-30 cm layer and dropped to 0.34-0.66% in the 30-60 cm layer and then to less than 0.1% in the 60-90 cm layer with the exception of the HYZ.

Table 4 Soil texture, soil organic carbon (SOC), lower limit, drained upper limit, total available water.

Zone	Depth (cm)	Clay (%)	Silt (%)	Sand (%)	SOC (%)	Lower limit (cm/cm)	Drained upper limit (cm/cm)	Total available water (cm/cm)
	0-30	13.20	39.70	47.10	0.95	0.09	0.28	0.19
HYZ	30-60	14.37	42.68	42.95	0.66	0.10	0.25	0.15
	60-90	19.25	37.58	43.17	0.38	0.10	0.25	0.15
	0-30	13.85	30.87	55.28	0.94	0.11	0.26	0.15
MYZ	30-60	22.16	30.90	46.94	0.34	0.11	0.26	0.15
	60-90	25.71	34.64	39.64	0.07	0.11	0.26	0.15
	0-30	14.35	38.68	46.97	0.92	0.12	0.28	0.16
LYZ	30-60	21.35	42.61	36.04	0.34	0.11	0.27	0.16
	60-90	25.67	41.89	32.44	0.05	0.11	0.27	0.17
	0-30	14.82	34.06	51.13	0.98	0.10	0.27	0.17
UYZ	30-60	18.74	35.61	45.65	0.52	0.11	0.27	0.16
	60-90	25.12	39.75	35.14	0.05	0.11	0.27	0.16

The simulations allowed to evaluate the effect of the different N fertilization levels in terms of spring barley grain yield (kg ha⁻¹), N-NO₃ leaching (kg ha⁻¹) and N-N₂O emissions (g ha⁻¹).

In the HYZ, the simulation outputs showed an high variability in relation to the N input for the 0N treatment (65% CV) with an average grain yield of 1109 kg ha⁻¹. The higher grain yield stability was observed for the 60N treatment (CV 12%) with an average grain yield of 5979 kg ha⁻¹.

As expected, the N leaching increased with the level of N input up to 11.3 kg ha⁻¹ with 140N, but the lowest values were simulated for treatments lower than 40 N ($3.1 \div 2.9 \text{ kg ha}^{-1}$).

The simulated emissions showed a similar trend, with minimum values of 0.02 g ha⁻¹ for the 0 N treatment up to 0.67 g ha⁻¹ for the 140N treatment.

The % variation vs. 120N of N-N₂O emissions, N-NO₃ leaching and grain yield in the HYZ (Fig. 19) revealed that reducing N fertilization of some 17% (100N vs 120N) crop yield would decrease of 2% while N2O emission by 27% and N leaching by 22% in the HYZ. In the HYZ, with a fertilization rate of 80 N (-33%) the grain yield decreased on average by only 5%, while the N leached and the N₂O emitted decreased by 41% and 50% respectively. A similar behaviour was observed on all MZs. These outputs are useful to optimize N fertilization in relation either to N₂O emissions or N leached per unit grain yield or per unit fertilization rate.

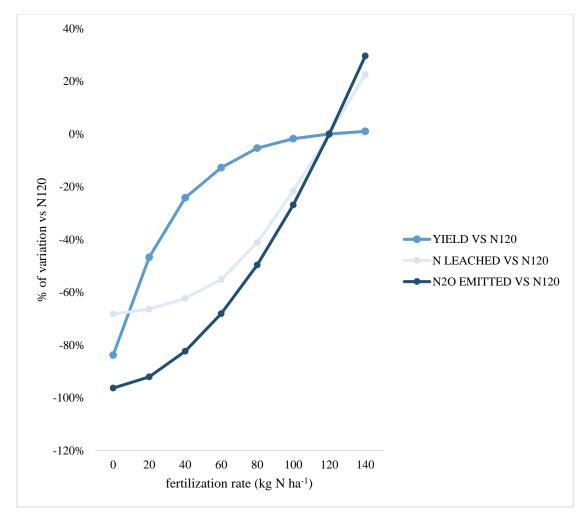


Figure 14 Relative effect for each N fertilization level in HYZ.

We observed similar trends in the MYZ in terms of grain yield variability (highest at 0N, lowest at 6160N), N leaching, which was highest (12.9 kg ha-1 N-NO₃) for 140N and lowest (3.0 kg ha⁻¹) for 20N. The simulated N2O emissions showed a trend similar to that of N leached, being lowest (0.03 kg ha⁻¹ N-N₂O) for the 0 N treatment up to 0.64 kg ha⁻¹ N-N₂O for the 140N treatment.

In the MYZ the reduction of the fertilization rate of 33% (80N) decreased grain yield by 4%, while the N leached and the N_2O emitted are reduced by 41% and 48% respectively.

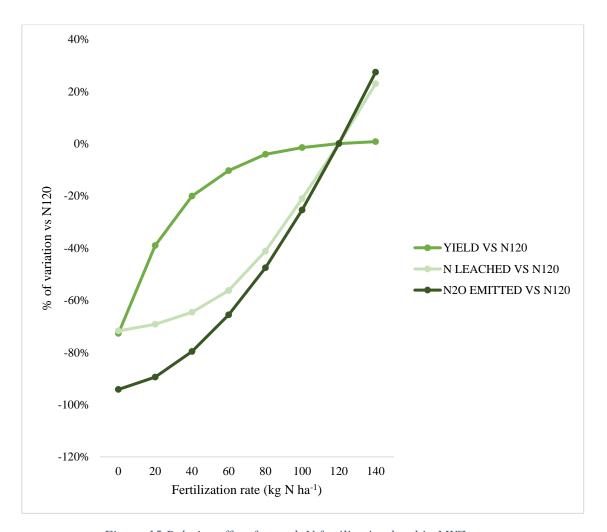


Figure 15 Relative effect for each N fertilization level in MYZ

In the LYZ we observed a lower grain yield (479 kg ha⁻¹) with higher variability for the 0N treatment (48% CV) with an average grain yield of 479, highest stability for the 40N treatment (CV 12%) with an average grain yield of 4834 kg ha⁻¹. The highest N leaching was simulated for the 140N rate (7.87 kg ha⁻¹), the lowest with 60 N (< 2.07 kg ha⁻¹). The simulated emissions showed a trend similar to that of N leached, with minimum values of 0.01 kg ha⁻¹ for the 0 N treatment and 0.78 kg ha⁻¹ for the 140N treatment.

In the LYZ, a reduction of 33% of the N rate led to -51% of N-NO $_3$ leaching or N-N $_2$ O emissions (Fig. 16).

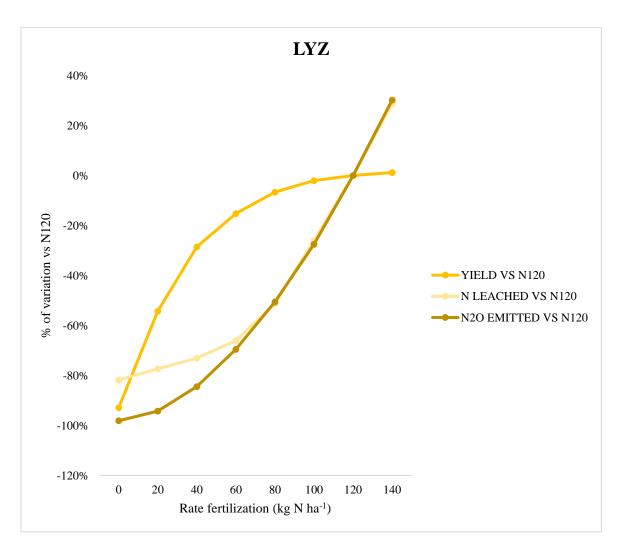


Figure 16 Relative effect for each N fertilization level in LYZ.

In the UYZ, similarly to what found in the other MZs, the highest grain yield variability was observed with the 0N treatment (33% CV) with an average grain yield of 1717 kg ha⁻¹, the lowest for the 40N treatment (CV 11%) with an average grain yield of 5468 kg ha⁻¹.

The highest leaching was observed with the highest level of N input (10.6 kg ha⁻¹ with 140N), the lowest at 20 N (< 2.56 kg ha⁻¹). The simulated emissions showed a similar trend, with minimum values of 0.026 kg ha⁻¹ for the 0 N treatment up to 0.88 kg ha⁻¹ for 140N.

In the LYZ, a reduction of 33% of the N fertilization rate led to a decrease of grain yield of only 4%, while the leached N-NO₃ and N-N2O decreased by 42% and 49% respectively.

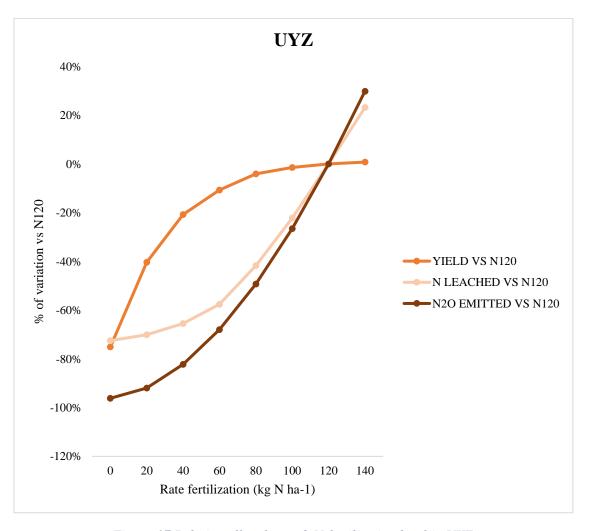


Figure 17 Relative effect for each N fertilization level in UYZ.

Drainage and N leaching data were also combined to quantify the potential nitrate N concentration (mg L^{-1}) in the percolation water. Drainage was similar in all treatments with lowest values in the LYZ and 0N treatment (277 mm) and highest in the MYZ at the 140N treatment (300 mm). The concentration of leached N showed an increasing trend with increasing N fertilization rate, ranging from 0.6 mg L^{-1} N-NO₃ to 4.3 mg L^{-1} N-NO₃. These values are lower than the maximum threshold identified by the EU for the nitrates directive, according to which the concentration of 11.3 mg L^{-1} N-NO₃ cannot be exceeded in drinking water.

Table 5 Spring barley grain yield, N leached and N_2O emissions for 120 N (business as usual fertilization in Scotland) and 80N (selected treatment)

N (kg N ha ⁻¹)	Zone	Yield (kg DM ha ⁻¹)		N leached (kg N ha ⁻¹)		N ₂ O emitted (g N-N ₂ O ha ⁻¹)	
		Mean	Dev. St.	Mean	Dev. St.	Mean	Dev. St.
120	113/7	6852	± 951	9.19	± 9.45	516.9	± 280
80	HYZ	6485	± 816	5.41	± 4.7	260.5	± 150
120	MYZ.	6835	± 985	10.51	± 10.67	500.1	± 320
80	NIYZ	6557	\pm 847	6.18	± 5.5	262.4	± 170
120	LYZ	6765	±967	6.11	± 7.51	601.3	± 270
80	LYZ	6312	±767	2.98	± 3.32	297	± 140
120	# 1 % 7/7	6898	± 942	8.58	± 9.29	680.4	± 290
80	UYZ	6616	± 811	5	± 4.55	345.2	± 160

The following Figures (18, 19, 20 and 21) show how the yield decreases with decreasing N fertilization rate, as is for the leached N quantity and the N_2O emissions. However the three trends follow a different pattern, which indicates that substantial reduction in the level of N fertilization would result in small decrease of grain yield but relevant decrease in N_2O emissions and NO_3 leaching.

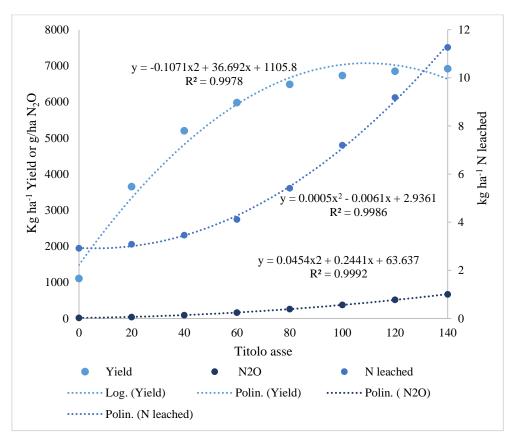


Figure 18 Regressions between N fertilization rates and grain yield, N leaching and N_2O emissions simulated by DSSAT for spring barley in the HYZ.

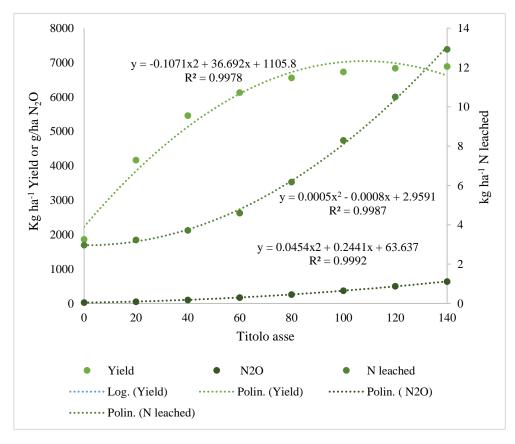


Figure 19 Regressions between N fertilization rates and grain yield, N leaching and N_2O emissions simulated by DSSAT for spring barley in the MYZ.

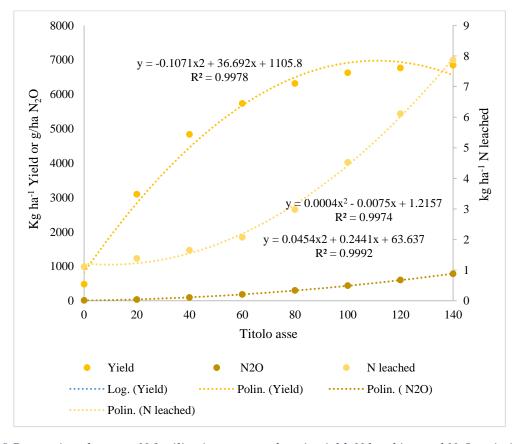


Figure 20 Regressions between N fertilization rates and grain yield, N leaching and N_2O emissions simulated by DSSAT for spring barley in the LYZ..

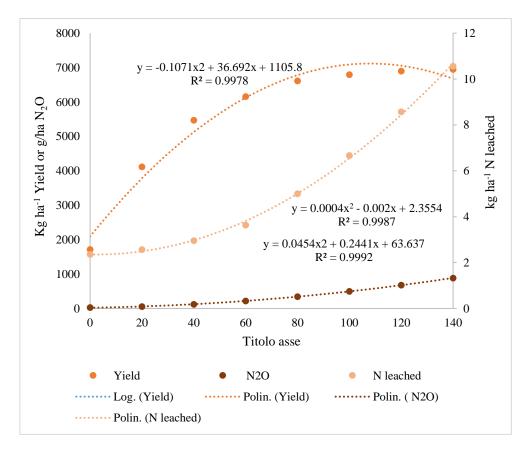


Figure 21 Regressions between N fertilization rates and grain yield, N leaching and N₂O emissions simulated by DSSAT for spring barley in the UYZ.

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6. Conclusions

In conclusion, DSSAT proved to be an effective tool for the simulation of the spring barley crop system in Scotland, as shown by the good results obtained in the calibration of the *Concerto* cultivar at the experimental site of the James Hutton Institute. The model's outputs were useful to study the space time variability associated respectively to soil and weather variations the different fertilization management and to evaluate the potential environmental implications. Furthermore, it was possible to simulate different quantitative responses to different levels of nitrogen inputs to optimize agronomic inputs and evaluate the effectiveness in terms of yield and nutrient loss as N₂O emissions or NO₃ leaching.

The model showed clearly that a substantial (-33%) reduction in N fertilization vs. the business as usual in Scotland (120N, can provide great benefits in terms of reduction of N leaching and N gaseous emissions with negligible (<5%) grain yield reductions. Furthermore, given the standards required by the malt industry, a reduction of the N fertilization rate can contribute to improve the malt quality by reducing its protein content. Given the relatively homogeneous field conditions in terms of soil types, we did not observe substantial improvements in terms of N use efficiency by optimizing N rate using precision farming technologies.

However, further studies would be needed to investigate the effects of N fertilization and its spatial distribution in terms of grain quality and the potential of precision fertilization technologies under more variable field conditions.

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